



## Author index to volume 202

Aardema, T.G., N.A.A.J. van Asten, J.P.J. Driessen, E.J.D. Vredenbregt and H.C.W.	
Beijerinck, Excitation transfer in collisions of Kr{4p <sup>5</sup> 5p; <sup>3</sup> D <sub>3</sub> } with N <sub>2</sub> molecules	202 (1996) 377
Adamsky, H., see Atanasov, M.	202 (1996) 155
Agostini, G., C. Corvaja and L. Pasimeni, EPR studies of the excited triplet states of C <sub>60</sub> O	
and C <sub>60</sub> C <sub>2</sub> H <sub>4</sub> N(CH <sub>3</sub> ) fullerene derivatives and C <sub>70</sub> in toluene and polymethylmethacry-	
late glasses and as films	202 (1996) 349
Allman, S.L., see Zhu, Y.F.	202 (1996) 175
Altmann, R.B., L. Kador and D. Haarer, Dipole moment differences of polar dyes in	
polymeric matrices: Stark effect and photochemical hole burning. II	202 (1996) 167
Armstrong, D.A., see Yu, D.	202 (1996) 243
Atanasov, M., H. Adamsky and D. Reinen, Ligand field analysis of Mn5+ in tetra-oxo	
coordination	202 (1996) 155
Baltzer, P., B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A. MacDonald,	
M.A. Hayes, P. Tomasello and W. von Niessen, An experimental and theoretical study	
of the valence shell photoelectron spectrum of carbon disulphide	202 (1996) 185
Bartocci, G., U. Mazzucato and A. Spalletti, Spectral and photophysical properties of	,
trans-2-styrylanthracene rotamers, derived by kinetic fluorescence analysis. A compari-	
son with the results obtained by statistical procedures	202 (1996) 367
Beijerinck, H.C.W., see Aardema, T.G.	202 (1996) 377
Bergmann, F., see Lorenz, W.	202 (1996) 39
Billing, G.D., see Gross, A.	202 (1996) 321
Birlirakis, N., see Lampre, I.	202 (1996) 107
Borchert, I., see Eschrich, I.	202 (1996) 211
Bosch, E., see Bouvier, A.J.	202 (1996) 139
Bougeard, D., see Ermoshin, V.A.	202 (1996) 53
Bouvier, A., see Bouvier, A.J.	202 (1996) 139
Bouvier, A.J., E. Bosch and A. Bouvier, Isotopic effects in the ground state of the	
non-symmetrical isotopomers of CuCl <sub>2</sub>	202 (1996) 139
Brillante, A., see Della Valle, R.G.	202 (1996) 231
Chakraborty, A., see Guchhait, N.	202 (1996) 387
Chen, C.H., see Zhu, Y.F.	202 (1996) 175
Chen, Jh., see Mao, Xa.	202 (1996) 357
Chen, LB., see Pan, YL.	202 (1996) 277
Chowdhury, M., see Guchhait, N.	202 (1996) 387
Corvaja, C., see Agostini, G.	202 (1996) 349
Cullen, J., Generalized valence bond solutions from a constrained coupled cluster method	202 (1996) 217

Della Valle, R.G., E. Venuti and A. Brillante, Quasi harmonic lattice dynamics: the phase	
diagram of benzene	202 (1996) 231
Diercksen, G.H.F., see Martin, I.	202 (1996) 307
Driessen, J.P.J., see Aardema, T.G.	202 (1996) 377
Erickson, R., Simulation of ENDOR spectra of radicals with anisotropic hyperfine and	
nuclear quadrupolar interactions in disordered solids Ermoshin, V.A., K.S. Smirnov and D. Bougeard, Ab initio generalized valence force field	202 (1996) 263
for zeolite modelling. 1. Siliceous zeolites Eschrich, I., C. Ruth, L. Ziegeler and I. Borchert, Influence of the molecular environment	202 (1996) 53
on the hyperfine interaction of <sup>111</sup> Cd ions in gaseous radioactive <sup>111</sup> InI <sub>3</sub>	202 (1996) 211
Felder, P., see Frey, J.G.	202 (1996) 397
Frey, J.G. and P. Felder, Photodissociation of CS <sub>2</sub> at 193 nm investigated by polarised	
photofragment translational spectroscopy	202 (1996) 397
Fujimura, Y., see Kato, T.	202 (1996) 95
Fukumoto, K., N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa,	
Infrared and Raman spectra of N-chloromethylamine	202 (1996) 253
Garrett, W.R., see Zhu, Y.F.	202 (1996) 175
Gatteschi, D. and B.S. Tsukerblat, Symmetry breaking and effective motional averaging in	202 (1))0) 1/3
double triangular clusters with exchange and electron transfer effects	202 (1996) 25
Gislason, E.A., see Song, JB.	202 (1996) 1
Gole, J.L., see Pugh, J.V.	202 (1996) 129
Gross, A. and G.D. Billing, Semiclassical treatment of molecular vibrational energy	202 (1))0) 12)
transfer in collision between vibrationally excited O <sub>3</sub> and Ar	202 (1996) 321
Guchhait, N., D. Majumdar, A. Chakraborty, D. Nath and M. Chowdhury, Low-frequency	202 (1770) 521
vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetrahydroquinoline in	
supersonic jet	202 (1996) 387
Haarer, D., see Altmann, R.B.	202 (1996) 167
Hamada, Y., see Fukumoto, K.	202 (1996) 253
Handschuh, M., see Lorenz, W.	202 (1996) 39
Hayes, M.A., see Baltzer, P.	202 (1996) 185
Hirakawa, A.Y., see Fukumoto, K.	202 (1996) 253
Hogreve, H., Theoretical study of the low-lying electronic spectrum of C <sub>2</sub> <sup>2+</sup>	202 (1996) 63
Holland, D.M.P., see Baltzer, P.	202 (1996) 185
Kador, L., see Altmann, R.B.	202 (1996) 167
Karlsson, L., see Baltzer, P.	202 (1996) 185
Karwowski, J., see Martin, I.	202 (1996) 307
Kato, T. and Y. Fujimura, Intermolecular interaction-induced quantum beats in femtosec-	
ond time-resolved light scattering from molecules: photon-polarization and inhomogeneous effects	202 (1996) 95
	202 (1996) 95
Kirkpatrick, C.C., see Viehland, L.A.	202 (1990) 283
Lampre, I., D. Markovitsi, N. Birlirakis and M. Veber, Dimerisation processes of triaryl	
pyrylium salts	202 (1996) 107
Lavin, A.C., see Martin, I.	202 (1996) 307

Lee, KW., see Park, SJ.	202 (1996) 15
Li, FM., see Pan, YL.	202 (1996) 277
Lorenz, W., M. Handschuh, F. Bergmann and D. Mayer, Nonequilibrium Fermi energy	202 (1990) 277
characteristics of n- and p-semiconductor electrodes under dark and photocurrents up to	
large band bending	202 (1996) 39
Lundqvist, M., see Baltzer, P.	202 (1996) 185
Euroqvisi, N.i., See Euroei, 1.	202 (1770) 103
MacDonald, M.A., see Baltzer, P.	202 (1996) 185
Majumdar, D., see Guchhait, N.	202 (1996) 387
Mao, Xa. and Jh. Chen, Radiation damping effects in solvent preirradiation experiments	
in NMR	202 (1996) 357
Markovitsi, D., see Lampre, I.	202 (1996) 107
Martin, I., A.C. Lavin, M. Velasco, M.O. Martin, J. Karwowski and G.H.F. Diercksen,	
Quantum defect orbital study of electronic transitions in Rydberg molecules: ammonium	
and fluoronium radicals	202 (1996) 307
Martin, M.O., see Martin, I.	202 (1996) 307
Masuko, Ei., see Fukumoto, K.	202 (1996) 253
Mayer, D., see Lorenz, W.	202 (1996) 39
Mazzucato, U., see Bartocci, G.	202 (1996) 367
Nath, D., see Guchhait, N.	202 (1996) 387
Ouillon, R., see Turc, C.	202 (1996) 81
Pan, YL., YY. Zhao, LB. Chen, Y. Yin and FM. Li, Effect of pseudo-phonon side	
hole in laser-induced hole filling	202 (1996) 277
Park, SJ. and KW. Lee, Site selective electronic spectroscopy and ligand field analysis	
of sodium cis-bis(iminodiacetato)chromate(III)	202 (1996) 15
Pasimeni, L., see Agostini, G.	202 (1996) 349
Pawlikowski, M. and B. Rys, Solvent effects in CD spectra of molecules consisting of two	
identical chromophores	202 (1996) 149
Perrin, B., see Turc, C.	202 (1996) 81
Phillips, R.C., see Zhu, Y.F.	202 (1996) 175
Pugh, J.V., K.K. Shen, C.B. Winstead and J.L. Gole, Accessing a low-lying bound	
electronic state of the alkali oxides, LiO and NaO, using laser induced fluorescence	202 (1996) 129
Ranson, P., see Turc, C.	202 (1996) 81
	202 (1996) 243
Rauk, A., see Yu, D.	202 (1996) 243
Reinen, D., see Atanasov, M.	202 (1996) 133
Ruth, C., see Eschrich, I.	
Rys, B., see Pawlikowski, M.	202 (1996) 149
Shen, K.K., see Pugh, J.V.	202 (1996) 129
Shkrob, I.A. and A.D. Trifunac, Ionization and H abstraction in laser photolysis of TMPD.	
A time-resolved pulsed EPR study	202 (1996) 117
Smirnov, K.S., see Ermoshin, V.A.	202 (1996) 53
Song, JB. and E.A. Gislason, Theoretical study of the effect of reagent rotation on the	
reaction of $O + H_2(\nu, J)$	202 (1996) 1

Soper, A.K., Empirical potential Monte Carlo simulation of fluid structure Spalletti, A., see Bartocci, G.	202 (1996) 295 202 (1996) 367
Tomasello, P., see Baltzer, P.	202 (1996) 185
Trifunac, A.D., see Shkrob, I.A.	202 (1996) 117
Tsukerblat, B.S., see Gatteschi, D.	202 (1996) 25
Turc, C., B. Perrin, R. Ouillon and P. Ranson, Experimental, theoretical and numerical studies of line broadening by disorder: the CO vibrational transition in solid $\alpha$ -(CO-N <sub>2</sub> )	
alloy	202 (1996) 81
Utsunomiya-Tate, N., see Fukumoto, K.	202 (1996) 253
Van Asten, N.A.A.J., see Aardema, T.G.	202 (1996) 377
Veber, M., see Lampre, I.	202 (1996) 107
Velasco, M., see Martin, I.	202 (1996) 307
Venuti, E., see Della Valle, R.G.	202 (1996) 231
Viehland, L.A. and C.C. Kirkpatrick, Test of interaction potentials for rare gas-halide	
systems	202 (1996) 285
Von Niessen, W., see Baltzer, P.	202 (1996) 185
Vredenbregt, E.J.D., see Aardema, T.G.	202 (1996) 377
Wannberg, B., see Baltzer, P.	202 (1996) 185
Winstead, C.B., see Pugh, J.V.	202 (1996) 129
Yin, Y., see Pan, YL. Yu, D., D.A. Armstrong and A. Rauk, The structures and relative energies of formamide	202 (1996) 277
(H <sub>2</sub> NCHO) and radical ions H <sub>2</sub> NCHO <sup>++</sup> , H <sub>2</sub> NCOH <sup>++</sup> and H <sub>3</sub> NCO <sup>++</sup>	202 (1996) 243
Zhao, YY., see Pan, YL. Zhu, Y.F., S.L. Allman, R.C. Phillips, W.R. Garrett and C.H. Chen, Photophysics of the	202 (1996) 277
acetone 3p Rydberg states utilizing two-photon resonant ionization spectroscopy	202 (1996) 175
Ziegeler, L., see Eschrich, I.	202 (1996) 211

## Subject index to volume 202

## Methods

## Theoretical

Classical mechanics	
Theoretical study of the effect of reagent rotation on the reaction of $O + H_2(\nu, J)$ , JB. Song and E.A. Gislason	202 (1996)
Quantized field theory	
Site selective electronic spectroscopy and ligand field analysis of sodium cis-bis(iminodia-cetato)chromate(III), SJ. Park and KW. Lee	202 (1996) 1
Coupling schemes and perturbative treatments	
Symmetry breaking and effective motional averaging in double triangular clusters with exchange and electron transfer effects, D. Gatteschi and B.S. Tsukerblat	202 (1996) 2
Transport quantum mechanics	
Nonequilibrium Fermi energy characteristics of n- and p-semiconductor electrodes under dark and photocurrents up to large band bending, W. Lorenz, M. Handschuh, F. Bergmann and D. Mayer	202 (1996) 3
Equilibrium statistical mechanics	
Quasi harmonic lattice dynamics: the phase diagram of benzene, R.G. Della Valle, E. Venuti and A. Brillante	202 (1996) 23
Ab initio schemes for stationary properties	
Ab initio generalized valence force field for zeolite modelling. 1. Siliceous zeolites, V.A.	
Ermoshin, K.S. Smirnov and D. Bougeard	202 (1996) 53
Theoretical study of the low-lying electronic spectrum of $C_2^{2+}$ , H. Hogreve	202 (1996) 63
Generalized valence bond solutions from a constrained coupled cluster method, J. Cullen The structures and relative energies of formamide (H <sub>2</sub> NCHO) and radical ions H <sub>2</sub> NCHO <sup>++</sup> ,	202 (1996) 21
H <sub>2</sub> NCOH '+ and H <sub>3</sub> NCO '+, D. Yu, D.A. Armstrong and A. Rauk	202 (1996) 243
Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate,	
Ei. Masuko, Y. Hamada and A.Y. Hirakawa	202 (1996) 253
Computational and simulation methods	
Experimental, theoretical and numerical studies of line broadening by disorder: the CO vibrational transition in solid $\alpha$ -(CO-N <sub>2</sub> ) alloy, C. Turc, B. Perrin, R. Ouillon and P.	
Ranson	202 (1996) 81

Generalized valence bond solutions from a constrained coupled cluster method, J. Cullen Quasi harmonic lattice dynamics: the phase diagram of benzene, R.G. Della Valle, E.	202 (1996) 217
Venuti and A. Brillante The structures and relative energies of formamide (H <sub>2</sub> NCHO) and radical ions H <sub>2</sub> NCHO <sup>-+</sup> ,	202 (1996) 231
H <sub>2</sub> NCOH <sup>++</sup> and H <sub>3</sub> NCO <sup>++</sup> , D. Yu, D.A. Armstrong and A. Rauk Simulation of ENDOR spectra of radicals with anisotropic hyperfine and nuclear quadrupo-	202 (1996) 243
lar interactions in disordered solids, R. Erickson  Effect of pseudo-phonon side hole in laser-induced hole filling, YL. Pan, YY. Zhao,	202 (1996) 263
LB. Chen, Y. Yin and FM. Li	202 (1996) 277
Test of interaction potentials for rare gas-halide systems, L.A. Viehland and C.C.	202 (1006) 205
Kirkpatrick C. L. C. L. C. L. C. L. C. L. C. C. L. C.	202 (1996) 285
Empirical potential Monte Carlo simulation of fluid structure, A.K. Soper Quantum defect orbital study of electronic transitions in Rydberg molecules: ammonium and fluoronium radicals, I. Martin, A.C. Lavin, M. Velasco, M.O. Martin, J. Karwowski	202 (1996) 295
and G.H.F. Diercksen	202 (1996) 307
Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing	202 (1996) 321
Molecular dynamics and scattering theory	
Theoretical study of the effect of reagent rotation on the reaction of $O + H_2(\nu, J)$ , JB.	
Song and E.A. Gislason	202 (1996) 1
Intermolecular interaction-induced quantum beats in femtosecond time-resolved light scat-	
tering from molecules: photon-polarization and inhomogeneous effects, T. Kato and Y.	202 (1004) 05
Fujimura	202 (1996) 95
Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing	202 (1996) 321
Experimental	
Magnetic resonances	
Dimerisation processes of triaryl pyrylium salts, I. Lampre, D. Markovitsi, N. Birlirakis and	
M. Veber	202 (1996) 107
Ionization and H abstraction in laser photolysis of TMPD. A time-resolved pulsed EPR	202 (1770) 101
study, I.A. Shkrob and A.D. Trifunac	202 (1996) 117
Simulation of ENDOR spectra of radicals with anisotropic hyperfine and nuclear quadrupo-	202 (1550) 11.
lar interactions in disordered solids, R. Erickson	202 (1996) 263
EPR studies of the excited triplet states of C <sub>60</sub> O and C <sub>60</sub> C <sub>2</sub> H <sub>4</sub> N(CH <sub>3</sub> ) fullerene deriva-	
tives and C <sub>70</sub> in toluene and polymethylmethacrylate glasses and as films, G. Agostini,	202 (1996) 349
C. Corvaja and L. Pasimeni	202 (1990) 349
Radiation damping effects in solvent preirradiation experiments in NMR, Xa. Mao and Jh. Chen	202 (1996) 357
Infrared spectroscopy	
Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa	202 (1996) 253
Raman spectroscopy	
Experimental, theoretical and numerical studies of line broadening by disorder: the CO	
vibrational transition in solid $\alpha$ -(CO-N <sub>2</sub> ) alloy, C. Turc, B. Perrin, R. Ouillon and P.	
Ranson	202 (1996) 81
AMILIOUI	202 (1770) 01

Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa	202 (1996) 253
Visible and UV spectroscopy	
Dimerisation processes of triaryl pyrylium salts, I. Lampre, D. Markovitsi, N. Birlirakis and M. Veber	202 (1996) 107
Accessing a low-lying bound electronic state of the alkali oxides, LiO and NaO, using laser	
induced fluorescence, J.V. Pugh, K.K. Shen, C.B. Winstead and J.L. Gole	202 (1996) 129
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J.	202 (1006) 120
Bouvier, E. Bosch and A. Bouvier Solvent effects in CD spectra of molecules consisting of two identical chromophores, M.	202 (1996) 139
Pawlikowski and B. Rys	202 (1996) 149
Ligand field analysis of Mn <sup>5+</sup> in tetra-oxo coordination, M. Atanasov, H. Adamsky and D.	202 (1))0) 11)
Reinen	202 (1996) 155
Fluorescence spectroscopy	
Site selective electronic spectroscopy and ligand field analysis of sodium cis-bis(iminodia-	
cetato)chromate(III), SJ. Park and KW. Lee	202 (1996) 15
Dimerisation processes of triaryl pyrylium salts, I. Lampre, D. Markovitsi, N. Birlirakis and	
M. Veber	202 (1996) 107
Accessing a low-lying bound electronic state of the alkali oxides, LiO and NaO, using laser	
induced fluorescence, J.V. Pugh, K.K. Shen, C.B. Winstead and J.L. Gole	202 (1996) 129
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J.	202 (1006) 120
Bouvier, E. Bosch and A. Bouvier  Spectral and photophysical properties of trans-2-styrylanthracene rotamers, derived by kinetic fluorescence analysis. A comparison with the results obtained by statistical procedures, G. Bartocci, U. Mazzucato and A. Spalletti	202 (1996) 139 202 (1996) 367
Photoelectron and Auger spectroscopy	
An experimental and theoretical study of the valence shell photoelectron spectrum of	
carbon disulphide, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, P. Tomasello and W. von Niessen	202 (1006) 195
Holland, M.A. MacDonald, M.A. Hayes, P. Tomasello and W. von Niessen	202 (1996) 185
Laser methods	
Dipole moment differences of polar dyes in polymeric matrices: Stark effect and photo-	
chemical hole burning. II, R.B. Altmann, L. Kador and D. Haarer	202 (1996) 167
Photophysics of the acetone 3p Rydberg states utilizing two-photon resonant ionization	
spectroscopy, Y.F. Zhu, S.L. Allman, R.C. Phillips, W.R. Garrett and C.H. Chen	202 (1996) 175
Excitation transfer in collisions of Kr{4p <sup>5</sup> 5p; <sup>3</sup> D <sub>3</sub> } with N <sub>2</sub> molecules, T.G. Aardema,	202 (1006) 277
N.A.A.J. van Asten, J.P.J. Driessen, E.J.D. Vredenbregt and H.C.W. Beijerinck Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetra-	202 (1996) 377
hydroquinoline in supersonic jet, N. Guchhait, D. Majumdar, A. Chakraborty, D. Nath	
and M. Chowdhury	202 (1996) 387
Synchrotron spectroscopies	
An experimental and theoretical study of the valence shell photoelectron spectrum of	
carbon disulphide, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P.	202 (1006) 195
Holland, M.A. MacDonald, M.A. Hayes, P. Tomasello and W. von Niessen	202 (1996) 185

Coherent optical spectroscopy  Dinala mamort differences of polar dues in polymeric matrices. Stark effect and photo	
Dipole moment differences of polar dyes in polymeric matrices: Stark effect and photo- chemical hole burning. II, R.B. Altmann, L. Kador and D. Haarer	202 (1996) 167
Multiple resonance spectroscopy	
Simulation of ENDOR spectra of radicals with anisotropic hyperfine and nuclear quadrupo- lar interactions in disordered solids, R. Erickson	202 (1996) 263
Atomic and molecular beam techniques	
Excitation transfer in collisions of Kr{4p <sup>5</sup> 5p; <sup>3</sup> D <sub>3</sub> } with N <sub>2</sub> molecules, T.G. Aardema, N.A.A.J. van Asten, J.P.J. Driessen, E.J.D. Vredenbregt and H.C.W. Beijerinck Photodissociation of CS <sub>2</sub> at 193 nm investigated by polarised photofragment translational	202 (1996) 377
spectroscopy, J.G. Frey and P. Felder	202 (1996) 397
Time-resolved experiments	
Ionization and H abstraction in laser photolysis of TMPD. A time-resolved pulsed EPR study, I.A. Shkrob and A.D. Trifunac  Influence of the molecular environment on the hyperfine interaction of <sup>111</sup> Cd ions in	202 (1996) 117
gaseous radioactive <sup>111</sup> InI <sub>3</sub> , I. Eschrich, C. Ruth, L. Ziegeler and I. Borchert EPR studies of the excited triplet states of C <sub>60</sub> O and C <sub>60</sub> C <sub>2</sub> H <sub>4</sub> N(CH <sub>3</sub> ) fullerene deriva-	202 (1996) 211
tives and $C_{70}$ in toluene and polymethylmethacrylate glasses and as films, G. Agostini, C. Corvaja and L. Pasimeni	202 (1996) 349
Mass spectrometry	
Test of interaction potentials for rare gas-halide systems, L.A. Viehland and C.C. Kirkpatrick	202 (1996) 285
Measurement of macroscopic variables	
Nonequilibrium Fermi energy characteristics of n- and p-semiconductor electrodes under dark and photocurrents up to large band bending, W. Lorenz, M. Handschuh, F. Bergmann and D. Mayer	202 (1996) 39
Objects	
Bulk systems	
Gases	
Test of interaction potentials for rare gas-halide systems, L.A. Viehland and C.C. Kirkpatrick	202 (1996) 285
Supersonic beams	
Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetrahydroquinoline in supersonic jet, N. Guchhait, D. Majumdar, A. Chakraborty, D. Nath	202 (4024) 207
and M. Chowdhury  Photodissociation of CS <sub>2</sub> at 193 nm investigated by polarised photofragment translational	202 (1996) 387
spectroscopy, J.G. Frey and P. Felder	202 (1996) 397

Liquids neat	
Empirical potential Monte Carlo simulation of fluid structure, A.K. Soper	202 (1996) 295
Liquid mixtures and solutions	
Solvent effects in CD spectra of molecules consisting of two identical chromophores, M. Pawlikowski and B. Rys	202 (1996) 149
Radiation damping effects in solvent preirradiation experiments in NMR, Xa. Mao and Jh. Chen	202 (1996) 357
Spectral and photophysical properties of trans-2-styrylanthracene rotamers, derived by kinetic fluorescence analysis. A comparison with the results obtained by statistical procedures, G. Bartocci, U. Mazzucato and A. Spalletti	202 (1996) 367
Crystals	
Ab initio generalized valence force field for zeolite modelling. 1. Siliceous zeolites, V.A. Ermoshin, K.S. Smirnov and D. Bougeard	202 (1996) 53
Quasi harmonic lattice dynamics: the phase diagram of benzene, R.G. Della Valle, E. Venuti and A. Brillante	202 (1996) 231
-neat	
Site selective electronic spectroscopy and ligand field analysis of sodium cis-bis(iminodiacetato)chromate(III), SJ. Park and KW. Lee	202 (1996) 15
-mixed	
Experimental, theoretical and numerical studies of line broadening by disorder: the CO vibrational transition in solid $\alpha$ -(CO-N <sub>2</sub> ) alloy, C. Turc, B. Perrin, R. Ouillon and P. Ranson	202 (1996) 81
Polymers	
Dipole moment differences of polar dyes in polymeric matrices: Stark effect and photo- chemical hole burning. II, R.B. Altmann, L. Kador and D. Haarer	202 (1996) 167
Semiconductors	
Nonequilibrium Fermi energy characteristics of n- and p-semiconductor electrodes under dark and photocurrents up to large band bending, W. Lorenz, M. Handschuh, F. Bergmann and D. Mayer	202 (1996) 39
Thin films	
Effect of pseudo-phonon side hole in laser-induced hole filling, YL. Pan, YY. Zhao, LB. Chen, Y. Yin and FM. Li	202 (1996) 277
Low-dimensional materials	
Symmetry breaking and effective motional averaging in double triangular clusters with exchange and electron transfer effects, D. Gatteschi and B.S. Tsukerblat	202 (1996) 25
Microscopic systems	
Molecules (neutral and ionic)	
Influence of the molecular environment on the hyperfine interaction of <sup>111</sup> Cd ions in gaseous radioactive <sup>111</sup> InI <sub>3</sub> , I. Eschrich, C. Ruth, L. Ziegeler and I. Borchert	202 (1996) 211

Quantum defect orbital study of electronic transitions in Rydberg molecules: ammonium and fluoronium radicals, I. Martin, A.C. Lavin, M. Velasco, M.O. Martin, J. Karwowski and G.H.F. Diercksen  EPR studies of the excited triplet states of C <sub>60</sub> O and C <sub>60</sub> C <sub>2</sub> H <sub>4</sub> N(CH <sub>3</sub> ) fullerene derivatives and C <sub>70</sub> in toluene and polymethylmethacrylate glasses and as films, G. Agostini, C. Corvaja and L. Pasimeni	202 (1996) 307 202 (1996) 349
<ul> <li>-diatomic</li> <li>Theoretical study of the low-lying electronic spectrum of C<sub>2</sub><sup>2+</sup>, H. Hogreve</li> <li>Accessing a low-lying bound electronic state of the alkali oxides, LiO and NaO, using laser induced fluorescence, J.V. Pugh, K.K. Shen, C.B. Winstead and J.L. Gole</li> </ul>	202 (1996) 63 202 (1996) 129
Excitation transfer in collisions of Kr{4p <sup>5</sup> 5p; <sup>3</sup> D <sub>3</sub> } with N <sub>2</sub> molecules, T.G. Aardema, N.A.A.J. van Asten, J.P.J. Driessen, E.J.D. Vredenbregt and H.C.W. Beijerinck	202 (1996) 377
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier  Photophysics of the acetone 3p Rydberg states utilizing two-photon resonant ionization spectroscopy, Y.F. Zhu, S.L. Allman, R.C. Phillips, W.R. Garrett and C.H. Chen  An experimental and theoretical study of the valence shell photoelectron spectrum of carbon disulphide, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, P. Tomasello and W. von Niessen  Influence of the molecular environment on the hyperfine interaction of <sup>111</sup> Cd ions in gaseous radioactive <sup>111</sup> InI <sub>3</sub> , I. Eschrich, C. Ruth, L. Ziegeler and I. Borchert  The structures and relative energies of formamide (H <sub>2</sub> NCHO) and radical ions H <sub>2</sub> NCHO '+, H <sub>2</sub> NCOH '+ and H <sub>3</sub> NCO '+, D. Yu, D.A. Armstrong and A. Rauk  Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa  Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing  Photodissociation of CS <sub>2</sub> at 193 nm investigated by polarised photofragment translational spectroscopy, J.G. Frey and P. Felder	202 (1996) 139 202 (1996) 175 202 (1996) 185 202 (1996) 211 202 (1996) 243 202 (1996) 253 202 (1996) 321 202 (1996) 397
-aromatics  Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetra-hydroquinoline in supersonic jet, N. Guchhait, D. Majumdar, A. Chakraborty, D. Nath and M. Chowdhury  Molecular aggregates	202 (1996) 387
-dimers  Intermolecular interaction-induced quantum beats in femtosecond time-resolved light scattering from molecules: photon-polarization and inhomogeneous effects, T. Kato and Y. Fujimura  Dimerisation processes of triaryl pyrylium salts, I. Lampre, D. Markovitsi, N. Birlirakis and M. Veber  Solvent effects in CD spectra of molecules consisting of two identical chromophores, M. Pawlikowski and B. Rys	202 (1996) 95 202 (1996) 107 202 (1996) 149

-clusters	
Symmetry breaking and effective motional averaging in double triangular clusters with exchange and electron transfer effects, D. Gatteschi and B.S. Tsukerblat	202 (1996) 25
-complexes	
Ligand field analysis of Mn <sup>5+</sup> in tetra-oxo coordination, M. Atanasov, H. Adamsky and D. Reinen	202 (1996) 155
Free radicals (including hydronium and muonium)	
Theoretical study of the low-lying electronic spectrum of $C_2^{2+}$ , H. Hogreve Ionization and H abstraction in laser photolysis of TMPD. A time-resolved pulsed EPR	202 (1996) 63
study, I.A. Shkrob and A.D. Trifunac	202 (1996) 117
The structures and relative energies of formamide (H <sub>2</sub> NCHO) and radical ions H <sub>2</sub> NCHO <sup>++</sup> , H <sub>2</sub> NCOH <sup>++</sup> and H <sub>3</sub> NCO <sup>++</sup> , D. Yu, D.A. Armstrong and A. Rauk	202 (1996) 243
Simulation of ENDOR spectra of radicals with anisotropic hyperfine and nuclear quadrupo-	202 (1990) 243
lar interactions in disordered solids, R. Erickson	202 (1996) 263
Quantum defect orbital study of electronic transitions in Rydberg molecules: ammonium	
and fluoronium radicals, I. Martin, A.C. Lavin, M. Velasco, M.O. Martin, J. Karwowski and G.H.F. Diercksen	202 (1996) 307
Ions and charge carriers	
Influence of the molecular environment on the hyperfine interaction of <sup>111</sup> Cd ions in gaseous radioactive <sup>111</sup> InI <sub>3</sub> , I. Eschrich, C. Ruth, L. Ziegeler and I. Borchert	202 (1996) 211
Phenomena	
Molecular structure	
Theoretical study of the low-lying electronic spectrum of $C_2^{2+}$ , H. Hogreve	202 (1996) 63
Dimerisation processes of triaryl pyrylium salts, I. Lampre, D. Markovitsi, N. Birlirakis and	
M. Veber	202 (1996) 107
Generalized valence bond solutions from a constrained coupled cluster method, J. Cullen	202 (1996) 217
Vibrations and rotations of molecules	
Ab initio generalized valence force field for zeolite modelling. 1. Siliceous zeolites, V.A.	202 (1004) 52
	202 (1996) 53
Ermoshin, K.S. Smirnov and D. Bougeard	
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J.	
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier	202 (1996) 139
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J.	
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa Semiclassical treatment of molecular vibrational energy transfer in collision between	202 (1996) 139 202 (1996) 253
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing	202 (1996) 139
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetra-	202 (1996) 139 202 (1996) 253
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing	202 (1996) 139 202 (1996) 253
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetrahydroquinoline in supersonic jet, N. Guchhait, D. Majumdar, A. Chakraborty, D. Nath	202 (1996) 139 202 (1996) 253 202 (1996) 321
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier Infrared and Raman spectra of N-chloromethylamine, K. Fukumoto, N. Utsunomiya-Tate, Ei. Masuko, Y. Hamada and A.Y. Hirakawa Semiclassical treatment of molecular vibrational energy transfer in collision between vibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinoline and N-deuterotetrahydroquinoline in supersonic jet, N. Guchhait, D. Majumdar, A. Chakraborty, D. Nath and M. Chowdhury	202 (1996) 139 202 (1996) 253 202 (1996) 321

Symmetry breaking and effective motional averaging in double triangular clusters with	
exchange and electron transfer effects, D. Gatteschi and B.S. Tsukerblat	202 (1996) 25
Nonequilibrium Fermi energy characteristics of n- and p-semiconductor electrodes under	
dark and photocurrents up to large band bending, W. Lorenz, M. Handschuh, F.	
Bergmann and D. Mayer	202 (1996) 39
Theoretical study of the low-lying electronic spectrum of $C_2^{2+}$ , H. Hogreve	202 (1996) 63
Accessing a low-lying bound electronic state of the alkali oxides, LiO and NaO, using laser	202 (1990) 03
	202 (1996) 129
induced fluorescence, J.V. Pugh, K.K. Shen, C.B. Winstead and J.L. Gole	202 (1996) 129
Ligand field analysis of Mn <sup>5+</sup> in tetra-oxo coordination, M. Atanasov, H. Adamsky and D.	202 (1006) 155
Reinen	202 (1996) 155
An experimental and theoretical study of the valence shell photoelectron spectrum of	
carbon disulphide, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P.	
Holland, M.A. MacDonald, M.A. Hayes, P. Tomasello and W. von Niessen	202 (1996) 185
Generalized valence bond solutions from a constrained coupled cluster method, J. Cullen	202 (1996) 217
The structures and relative energies of formamide (H <sub>2</sub> NCHO) and radical ions H <sub>2</sub> NCHO <sup>++</sup> ,	
H <sub>2</sub> NCOH '+ and H <sub>3</sub> NCO '+, D. Yu, D.A. Armstrong and A. Rauk	202 (1996) 243
Simulation of ENDOR spectra of radicals with anisotropic hyperfine and nuclear quadrupo-	
lar interactions in disordered solids, R. Erickson	202 (1996) 263
Quantum defect orbital study of electronic transitions in Rydberg molecules: ammonium	
and fluoronium radicals, I. Martin, A.C. Lavin, M. Velasco, M.O. Martin, J. Karwowski	
and G.H.F. Diercksen	202 (1996) 307
and Gilli Pielensen	202 (1990) 507
Electric and magnetic managing	
Electric and magnetic properties	
Symmetry breaking and effective motional averaging in double triangular clusters with	202 (1004) 25
exchange and electron transfer effects, D. Gatteschi and B.S. Tsukerblat	202 (1996) 25
Dipole moment differences of polar dyes in polymeric matrices: Stark effect and photo-	()
chemical hole burning. II, R.B. Altmann, L. Kador and D. Haarer	202 (1996) 167
Radiation damping effects in solvent preirradiation experiments in NMR, Xa. Mao and	
Jh. Chen	202 (1996) 357
Optical activity	
Solvent effects in CD spectra of molecules consisting of two identical chromophores, M.	
Pawlikowski and B. Rys	202 (1996) 149
Molecular interactions	
Dipole moment differences of polar dyes in polymeric matrices: Stark effect and photo-	
chemical hole burning. II, R.B. Altmann, L. Kador and D. Haarer	202 (1996) 167
Test of interaction potentials for rare gas-halide systems, L.A. Viehland and C.C.	202 (1770) 107
Kirkpatrick	202 (1996) 285
Klikpatiick	202 (1990) 283
Spectral handshapes and intensities	
Spectral bandshapes and intensities	
Experimental, theoretical and numerical studies of line broadening by disorder: the CO	
vibrational transition in solid $\alpha$ -(CO-N <sub>2</sub> ) alloy, C. Turc, B. Perrin, R. Ouillon and P.	202 (1004) 01
Ranson	202 (1996) 81
Quantum defect orbital study of electronic transitions in Rydberg molecules: ammonium	
and fluoronium radicals, I. Martin, A.C. Lavin, M. Velasco, M.O. Martin, J. Karwowski	
and G.H.F. Diercksen	202 (1996) 307

Counting of electronic and muslom motion	
Coupling of electronic and nuclear motion  Solvent effects in CD spectra of molecules consisting of two ic  Pawlikowski and B. Rys	dentical chromophores, M. 202 (1996) 149
Energy transfer processes  Intermolecular interaction-induced quantum beats in femtosecontering from molecules: photon-polarization and inhomogeneous Fujimura	
Excitation transfer in collisions of Kr{4p <sup>5</sup> 5p; <sup>3</sup> D <sub>3</sub> } with N <sub>2</sub> n N.A.A.J. van Asten, J.P.J. Driessen, E.J.D. Vredenbregt and	nolecules, T.G. Aardema,
Molecular photophysical processes  An experimental and theoretical study of the valence shell per carbon disulphide, P. Baltzer, B. Wannberg, M. Lundqv	ist, L. Karlsson, D.M.P.
Holland, M.A. MacDonald, M.A. Hayes, P. Tomasello and W. EPR studies of the excited triplet states of C <sub>60</sub> O and C <sub>60</sub> C <sub>2</sub> H <sub>4</sub> tives and C <sub>70</sub> in toluene and polymethylmethacrylate glasses	N(CH <sub>3</sub> ) fullerene deriva-
C. Corvaja and L. Pasimeni Spectral and photophysical properties of trans-2-styrylanthrace kinetic fluorescence analysis. A comparison with the result	
procedures, G. Bartocci, U. Mazzucato and A. Spalletti Photodissociation of CS <sub>2</sub> at 193 nm investigated by polarised p	202 (1996) 367 hotofragment translational
spectroscopy, J.G. Frey and P. Felder  Intramolecular dynamics	202 (1996) 397
-vibrational energy redistribution (including vibrational dissocial Semiclassical treatment of molecular vibrational energy transvibrationally excited O <sub>3</sub> and Ar, A. Gross and G.D. Billing	
Luminescence spectra, yields and lifetimes  Site selective electronic spectroscopy and ligand field analysis of cetato)chromate(III), SJ. Park and KW. Lee	202 (1996) 15
Accessing a low-lying bound electronic state of the alkali oxides, induced fluorescence, J.V. Pugh, K.K. Shen, C.B. Winstead a Spectral and photophysical properties of trans-2-styrylanthrace kinetic fluorescence analysis. A comparison with the result	and J.L. Gole 202 (1996) 129 ene rotamers, derived by
procedures, G. Bartocci, U. Mazzucato and A. Spalletti	202 (1996) 367
Multiphoton phenomena  Photophysics of the acetone 3p Rydberg states utilizing two-ple spectroscopy, Y.F. Zhu, S.L. Allman, R.C. Phillips, W.R. Gar Low-frequency vibrations in S <sub>1</sub> states of tetrahydroquinol	rrett and C.H. Chen 202 (1996) 175 ine and N-deuterotetra-
hydroquinoline in supersonic jet, N. Guchhait, D. Majumdar, and M. Chowdhury	A. Chakraborty, D. Nath 202 (1996) 387
Reactions (including dissociation)	
<ul> <li>-gas phase</li> <li>Theoretical study of the effect of reagent rotation on the reaction</li> <li>Song and E.A. Gislason</li> </ul>	n of O + H <sub>2</sub> ( $\nu$ , $J$ ), JB. 202 (1996) 1

Influence of the molecular environment on the hyperfine interaction of <sup>111</sup> Cd ions in gaseous radioactive <sup>111</sup> InI <sub>3</sub> , I. Eschrich, C. Ruth, L. Ziegeler and I. Borchert	202 (1996) 211
-photochemical  Effect of pseudo-phonon side hole in laser-induced hole filling, YL. Pan, YY. Zhao,	
LB. Chen, Y. Yin and FM. Li	202 (1996) 277
Ionization (including Rydberg states)	
Ionization and H abstraction in laser photolysis of TMPD. A time-resolved pulsed EPR study, I.A. Shkrob and A.D. Trifunac	202 (1996) 117
Isotopic effects	
Isotopic effects in the ground state of the non-symmetrical isotopomers of CuCl <sub>2</sub> , A.J. Bouvier, E. Bosch and A. Bouvier	202 (1996) 139
Fluctuations and noise	
Intermolecular interaction-induced quantum beats in femtosecond time-resolved light scat- tering from molecules: photon-polarization and inhomogeneous effects, T. Kato and Y. Fujimura	202 (1996) 95
Thermodynamic and transport properties  Test of interaction potentials for rare gas-halide systems, L.A. Viehland and C.C.	
Kirkpatrick	202 (1996) 285
Structure of solids and liquids	
Quasi harmonic lattice dynamics: the phase diagram of benzene, R.G. Della Valle, E.	202 (4005) 224
Venuti and A. Brillante Empirical potential Monte Carlo simulation of fluid structure, A.K. Soper	202 (1996) 231 202 (1996) 295
Empirical potential Monte Carlo simulation of fluid structure, A.K. Soper	202 (1990) 293
Phase transitions	
Quasi harmonic lattice dynamics: the phase diagram of benzene, R.G. Della Valle, E. Venuti and A. Brillante	202 (1996) 231